

BetaShape and related studies

Nuclear Data Week 2020 – USNDP | Xavier Mougeot



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Outline

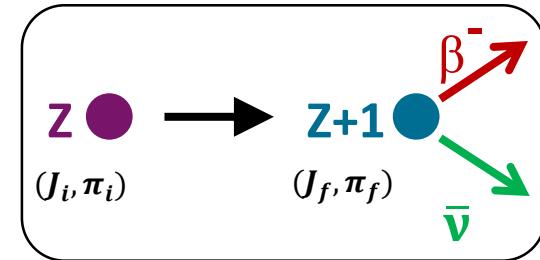
- Summary of the BetaShape formalism and status of the code
- Recent work about forbidden non-unique transitions with realistic nuclear structure
- Recent experimental work using silicon detectors
- Perspectives

BetaShape

Beta decay modelling

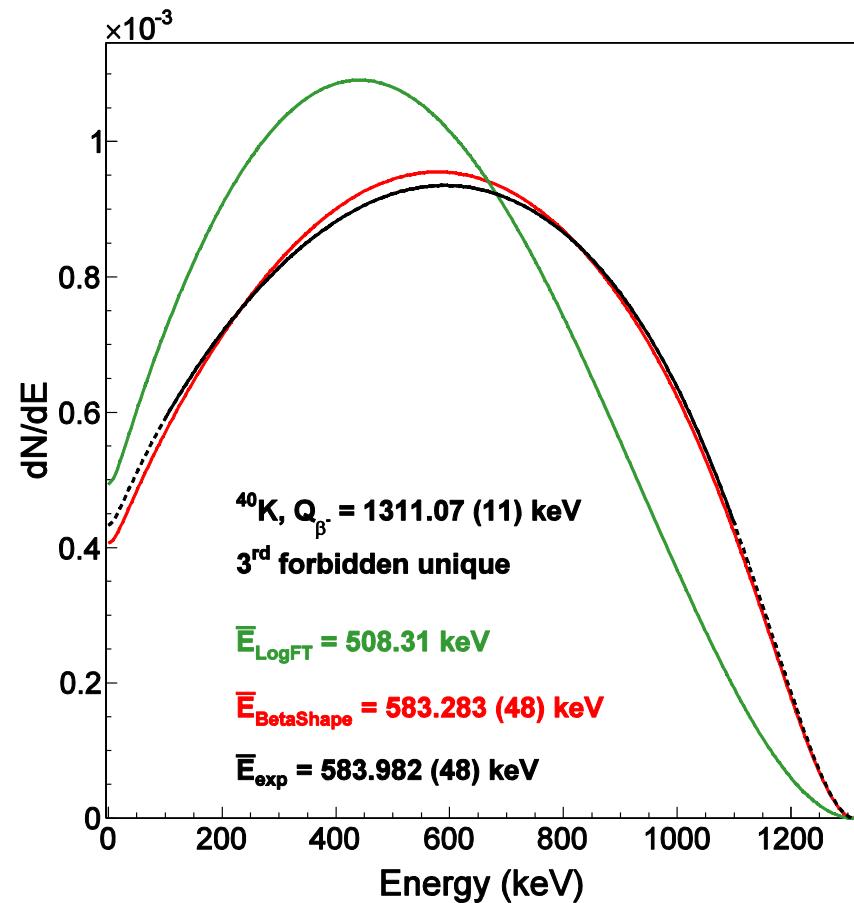
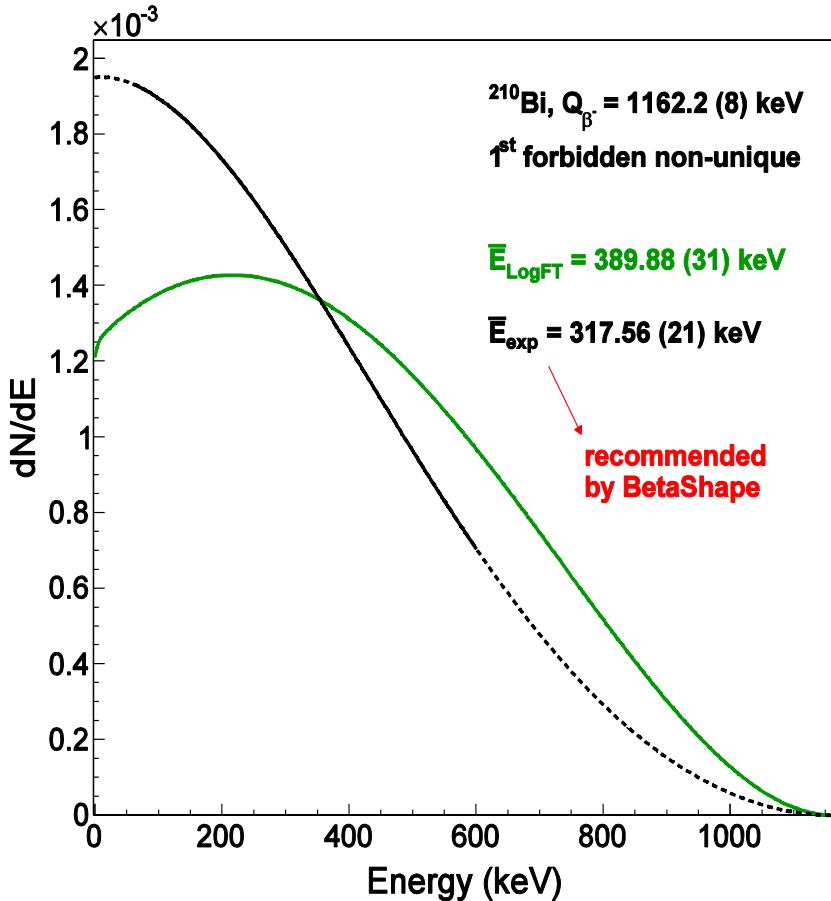
Beta spectrum

$$\frac{dN}{dW} \propto \begin{matrix} \text{Coulomb part} \\ \text{(Fermi function)} \end{matrix} \begin{matrix} p & W & q^2 & F_0 L_0 & C(W) \\ \text{Phase} & & & & \text{Shape} \\ \text{space} & & & & \text{factor} \end{matrix}$$



- Behrens and Bühring formalism
- Dirac equation solved numerically for beta particles (with spherical nucleus)
- Allowed and forbidden unique transitions
- Forbidden non-unique transitions with ξ approximation
- Bühring screening correction with Salvat's potentials
- Precise radiative corrections from Hardy's study of superallowed transitions
- Database of experimental shape factors (131 transitions)
- Propagation of uncertainties on Q-values and level energies
- Reads and writes to/from ENSDF files
- Provides beta and neutrino spectra for each transition, total spectrum for a radionuclide, mean energies, log ft values and report files

Examples of improved calculations



These two transitions are calculated as allowed by the LogFT program, which does not provide any beta spectrum.

Electron capture modelling

Total capture probability

$$\lambda_\varepsilon \propto \sum_{\kappa_x} n_{\kappa_x} C_{\kappa_x} q_{\kappa_x}^2 \beta_{\kappa_x}^2 B_{\kappa_x} \left(1 + \sum_{m,\kappa} P_{m\kappa} \right)$$

relative occupation number

ν momentum

shell quantum number

"shape" factor similar to $C(W)$ in β decay

amplitude of wave function

overlap and exchange corrections

shaking effects

+ hole effect (vacancy)
+ radiative corrections

Allowed and forbidden unique

→ no nuclear structure

If transition energy $\geq 2m_e$

→ competition with a β^+ transition

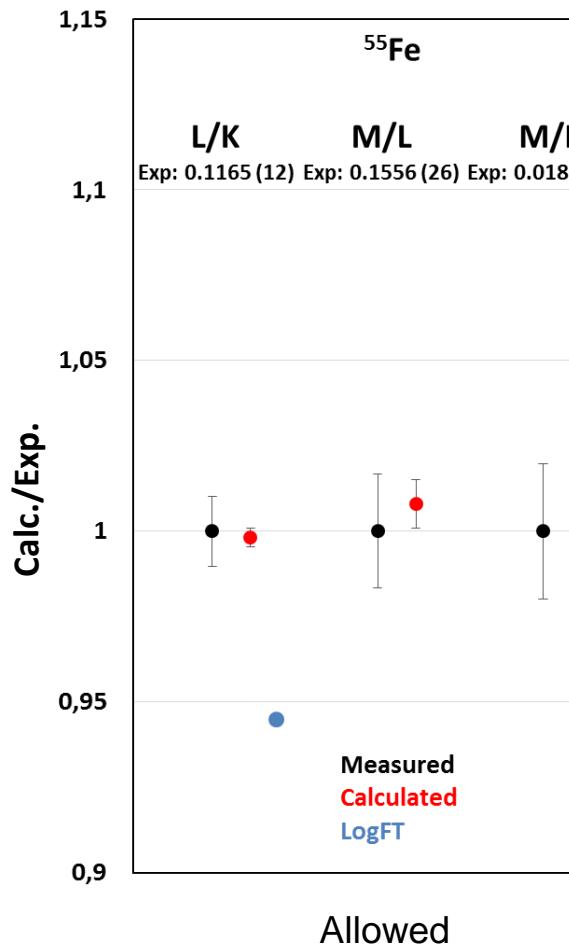
X. Mougeot, Appl. Radiat. Isot. 154, 108884 (2019)

Atomic wave functions

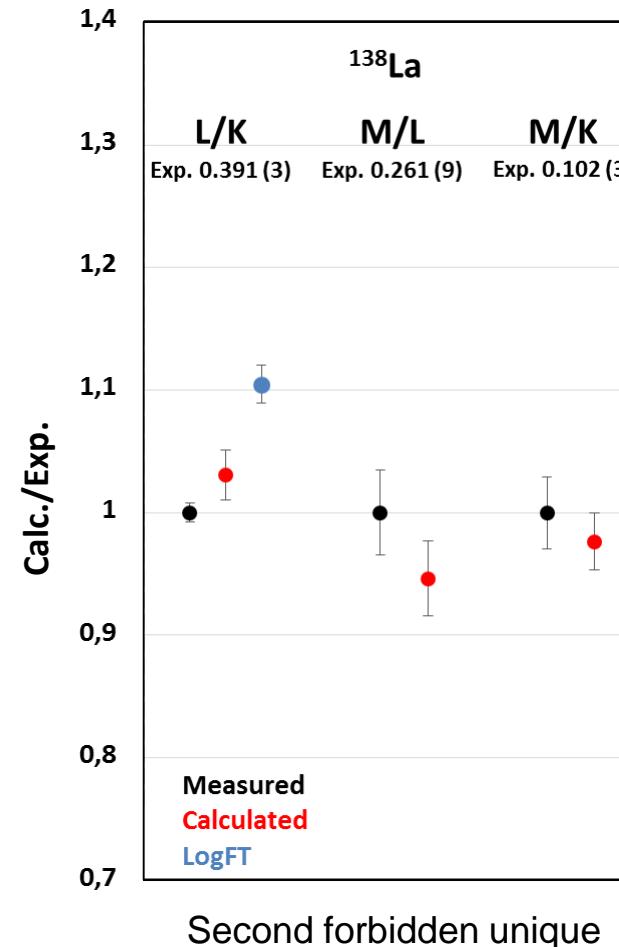
- Numerical solving of Dirac equation
- Forced convergence to relativistic DFT energies, with electron correlations

S. Kotochigova *et al.*, Phys. Rev. A 55, 191 (1997)

Comparison with measurements



J. Pengra *et al.*, Phys. Rev. C 5, 2007 (1972)
M. Loidl *et al.*, Appl. Radiat. Isot. 134, 395 (2018)

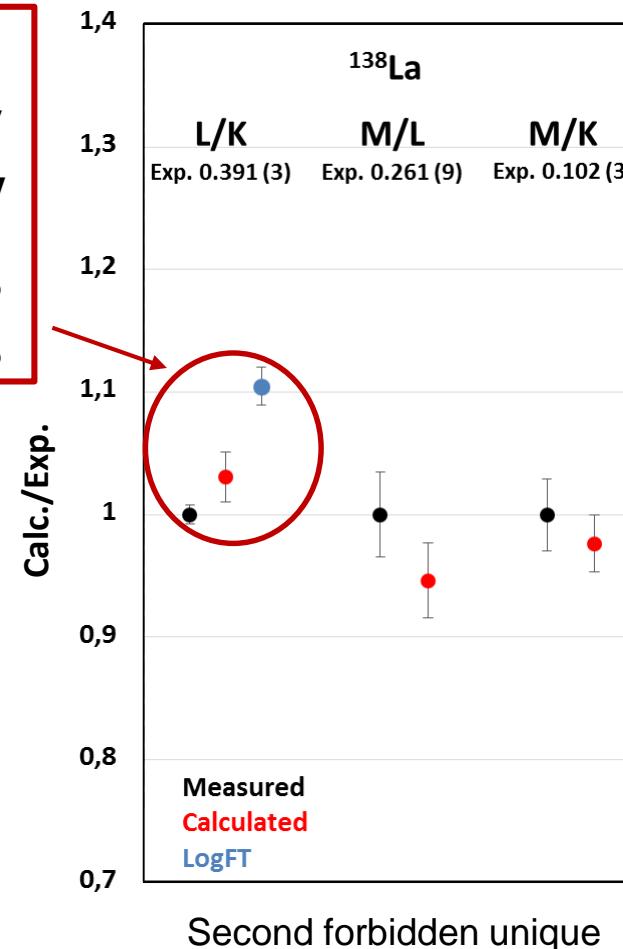
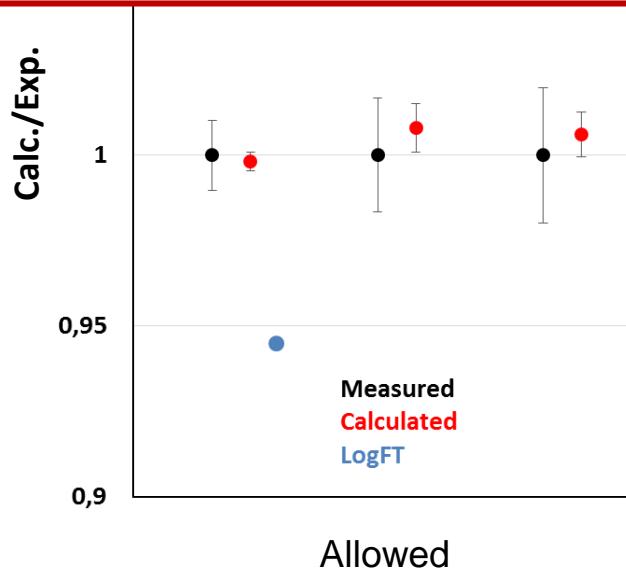


F. Quarati *et al.*, Appl. Radiat. Isot. 109, 172 (2016)

Comparison with measurements

New high-precision measurement of ^{138}La Q-values

- AME2016: $Q_{\varepsilon} = 1742(3)$ keV
- PRC 100 (2019) 014308: $Q_{\varepsilon} = 1748.41(34)$ keV
- Exp. L/K = 0.391 (3) $\Delta Q_{\varepsilon} < 0.4\%$
- Calc. L/K = 0.3913 (26) $\Delta(L/K)_{\text{calc.}} \sim 3\%$



J. Pengra *et al.*, Phys. Rev. C 5, 2007 (1972)
M. Loidl *et al.*, Appl. Radiat. Isot. 134, 395 (2018)

F. Quarati *et al.*, Appl. Radiat. Isot. 109, 172 (2016)

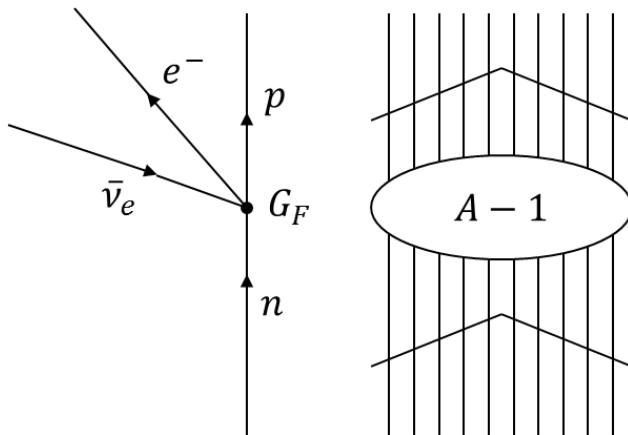
Recent work on theory

Theoretical shape factor

H. Behrens, W. Bühring, *Electron Radial Wave functions and Nuclear Beta Decay*, Oxford Science Publications (1982)

$$C(W_e) = \sum_{K k_e k_\nu} \lambda_{k_e} \left[M_K^2(k_e, k_\nu) + m_K^2(k_e, k_\nu) - \frac{2\mu_{k_e}\gamma_{k_e}}{k_e W_e} M_K(k_e, k_\nu) m_K(k_e, k_\nu) \right]$$

Multipole expansion of hadron and lepton currents. Calculation of shape factors, half-lives, branching ratios, log ft values.



Fermi theory

- Vertex of the weak interaction is assumed to be pointlike. No propagation of W^\pm boson.
- Effective coupling constant G_F .

Impulse approximation

- The nucleon is assumed to feel only the weak interaction.
- Other nucleons are spectators.

Forbidden non-unique transitions

Leading term for these transitions, simplifying the lepton current:

$$M_n(k_e, k_\nu) = K_n(pR)^{k_e-1}(qR)^{k_\nu-1} \left\{ -\sqrt{\frac{2n+1}{n}} \underbrace{^V F_{n,n-1,1}^{(0)}}_{\text{Relativistic matrix element}} - \frac{\alpha Z}{2k_e+1} \underbrace{^V F_{n,n,0}^{(0)}(k_e, 1, 1, 1)}_{\text{Relativistic matrix element}} \right.$$

$$\left. - \left[\frac{WR}{2k_e+1} + \frac{qR}{2k_\nu+1} \right] \underbrace{^V F_{n,n,0}^{(0)}}_{\text{Relativistic matrix element}} - \frac{\alpha Z}{2k_e+1} \sqrt{\frac{n+1}{n}} \underbrace{^A F_{n,n,1}^{(0)}(k_e, 1, 1, 1)}_{\text{Relativistic matrix element}} - \left[\frac{WR}{2k_e+1} - \frac{qR}{2k_\nu+1} \right] \sqrt{\frac{n+1}{n}} \underbrace{^A F_{n,n,1}^{(0)}}_{\text{Relativistic matrix element}} \right\}$$

Nuclear structure models are non-relativistic

→ Small component of nucleon wave function estimated from large (non-relativistic) component.

OR

→ **Conserved Vector Current (CVC) hypothesis**

- Comes from gauge invariance of the weak interaction.
- Relationships between non-relativistic and relativistic vector matrix elements.

Realistic nuclear structure

Nuclear state described as a **superposition of nucleon states**

$$\langle \xi_f J_f || T_\lambda || \xi_i J_i \rangle = \hat{\lambda}^{-1} \sum_{a,b} \langle a || T_\lambda || b \rangle \langle \xi_f J_f || [c_a^\dagger c_b]_\lambda || \xi_i J_i \rangle$$

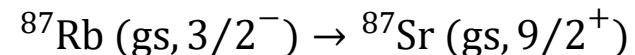
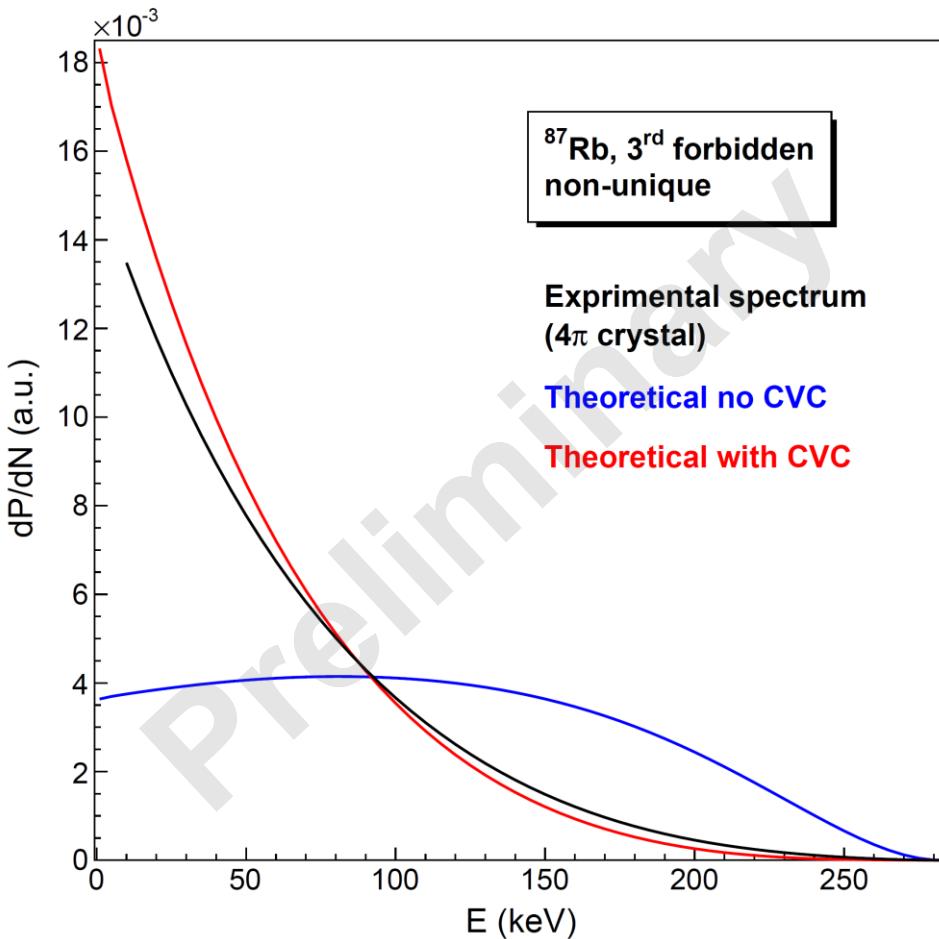
transition matrix element tensor rank single particle matrix element one-body transition density

The diagram illustrates the mathematical decomposition of a nuclear transition matrix element. It shows the expression $\langle \xi_f J_f || T_\lambda || \xi_i J_i \rangle = \hat{\lambda}^{-1} \sum_{a,b} \langle a || T_\lambda || b \rangle \langle \xi_f J_f || [c_a^\dagger c_b]_\lambda || \xi_i J_i \rangle$. Four arrows point from labels below to specific parts of the equation: 'transition matrix element' points to the overall bra-ket pair; 'tensor rank' points to the summation index a,b ; 'single particle matrix element' points to the term $\langle a || T_\lambda || b \rangle$; and 'one-body transition density' points to the term $\langle \xi_f J_f || [c_a^\dagger c_b]_\lambda || \xi_i J_i \rangle$.

One-body transition densities must be given by a nuclear structure model.

NushellX@MSU: spherical shell model, effective Hamiltonians fitted on nuclear data, widely used.

Preliminary study of ^{87}Rb



- Third forbidden non-unique transition
 - NushellX ^{56}Ni doubly magic core, jj44 model space, jj44b interaction
 - Preliminary measurement from the European MetroBeta project (4π RbGd_2Br_7 crystal)
- **CVC hypothesis mandatory for an accurate description of the spectrum**

Preliminary study of ^{36}Cl

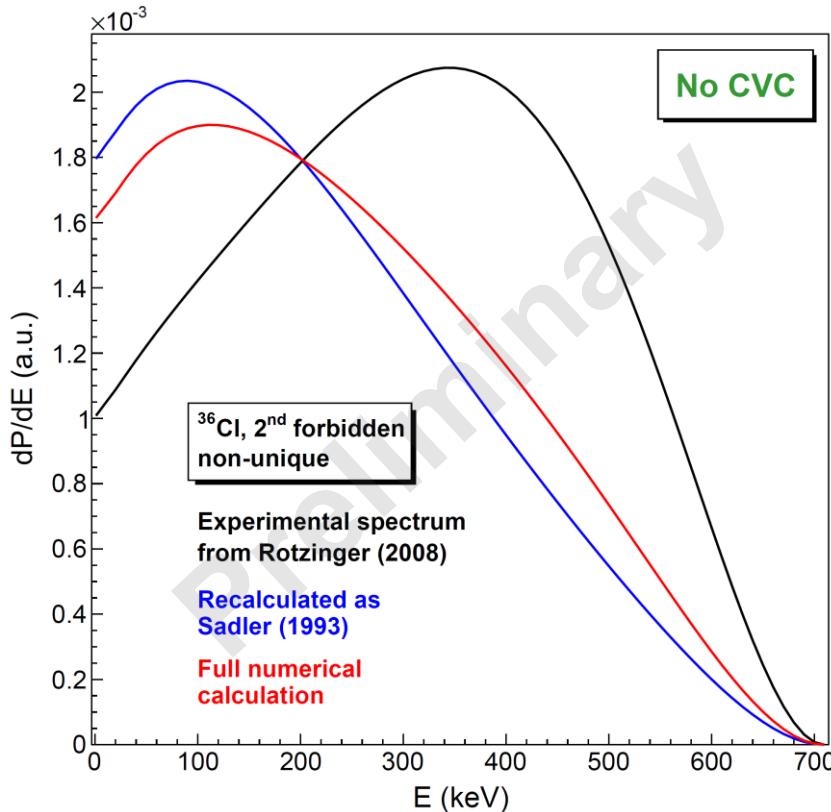
Precise measurement exists

Rotzinger et al., J. Low Temp.
Phys. 151, 1087 (2008)

Detailed theoretical study (with approximations)

Sadler, Behrens, Z. Phys. A 346, 25 (1993)

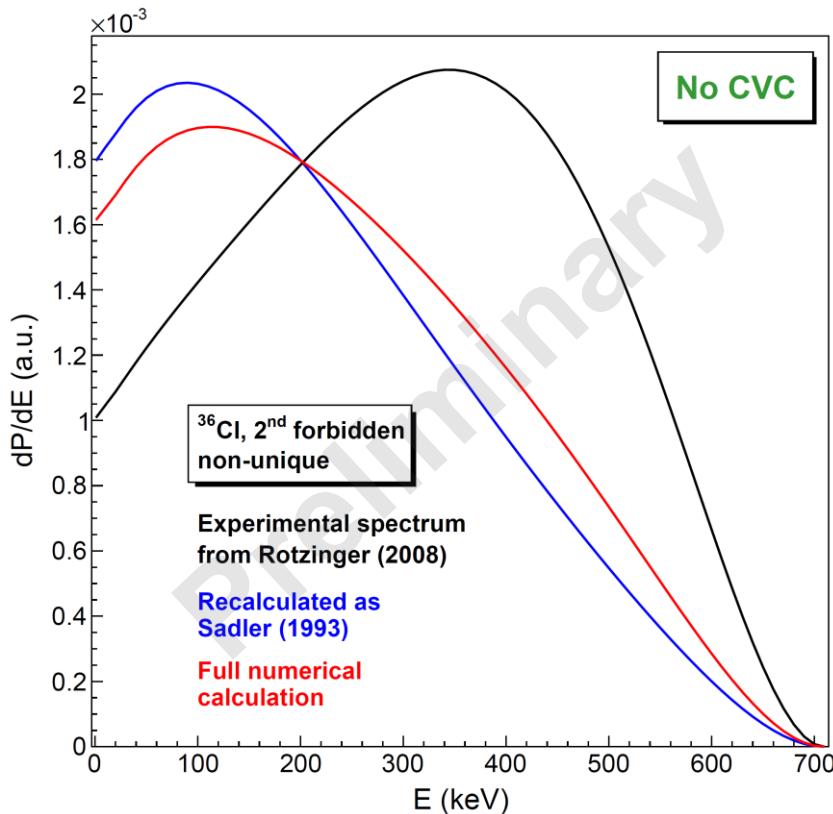
→ Matrix elements are correctly recalculated



Preliminary study of ^{36}Cl

Precise measurement exists

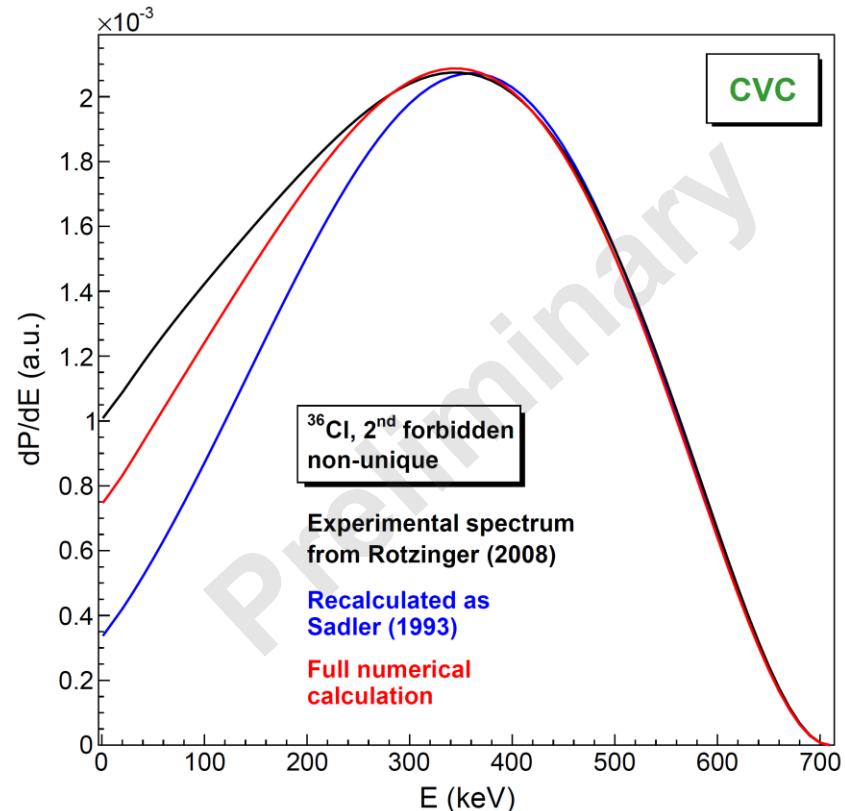
Rotzinger et al., J. Low Temp. Phys. 151, 1087 (2008)



Detailed theoretical study (with approximations)

Sadler, Behrens, Z. Phys. A 346, 25 (1993)

→ Matrix elements are correctly recalculated



→ CVC hypothesis mandatory + Influence of lepton current treatment

Reactor antineutrino anomaly

PHYSICAL REVIEW C **100**, 054323 (2019)

First-forbidden transitions in the reactor anomaly

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²*Department of Physics, University of Jyväskylä, P.O. Box 35, FI-40014 University of Jyväskylä, Finland*



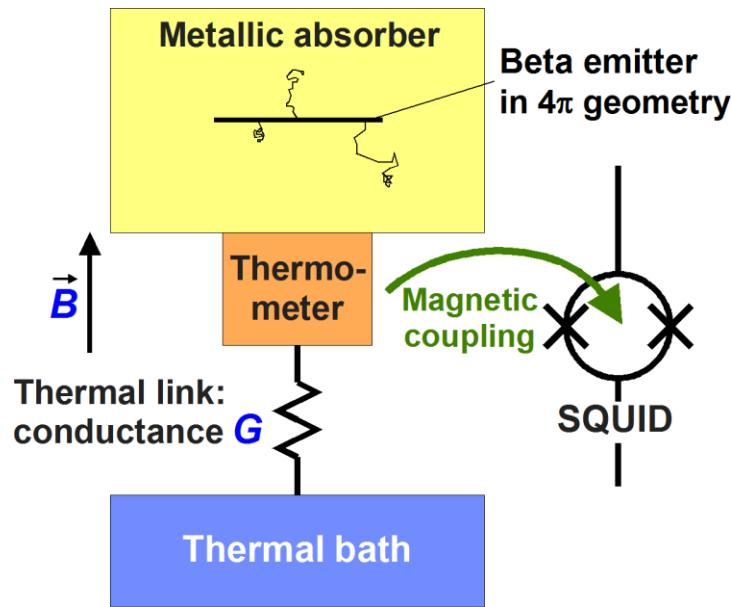
(Received 22 August 2019; published 20 November 2019)

We describe here microscopic calculations performed on the dominant forbidden transitions in reactor antineutrino spectra above 4 MeV using the nuclear shell model. By taking into account Coulomb corrections in the most complete way, we calculate the shape factor with the highest fidelity and show strong deviations from allowed approximations and previously published results. Despite small differences in the *ab initio* electron cumulative spectra, large differences on the order of several percent are found in the antineutrino spectra. Based on the behavior of the numerically calculated shape factors we propose a parametrization of forbidden spectra. Using Monte Carlo techniques we derive an estimated spectral correction and uncertainty due to forbidden transitions. We establish the dominance and importance of forbidden transitions in both the reactor anomaly and spectral shoulder analysis with their respective uncertainties. Based on these results, we conclude that a correct treatment of forbidden transitions is indispensable in both the normalization anomaly and spectral shoulder.

- Conclusion: first forbidden non-unique transitions could explain by themselves the reactor anomaly
- Drawbacks: **no account of CVC hypothesis**, simplified lepton current

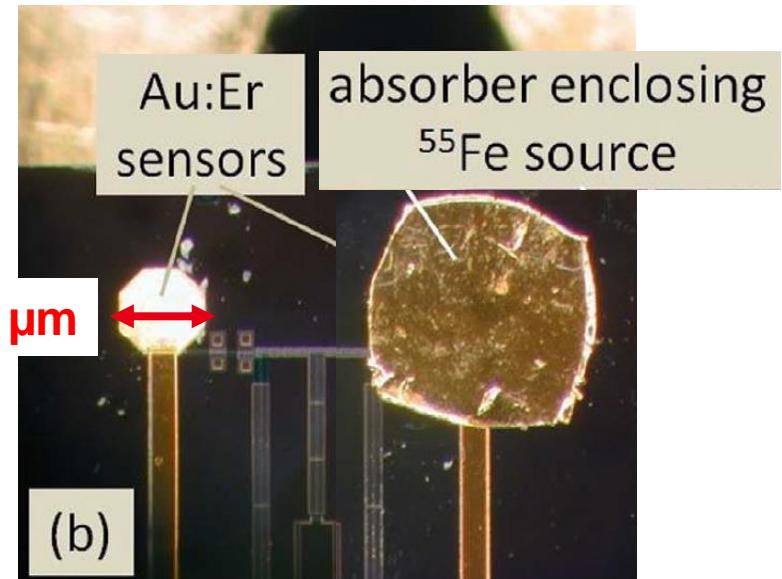
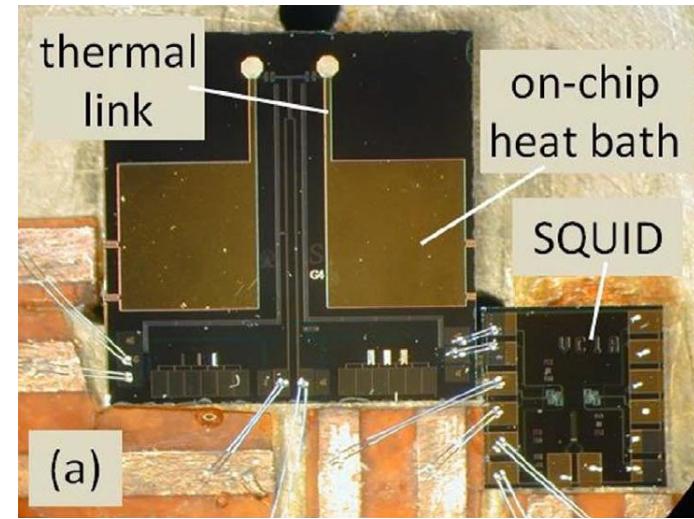
Recent work on experiments

Metallic magnetic calorimetry



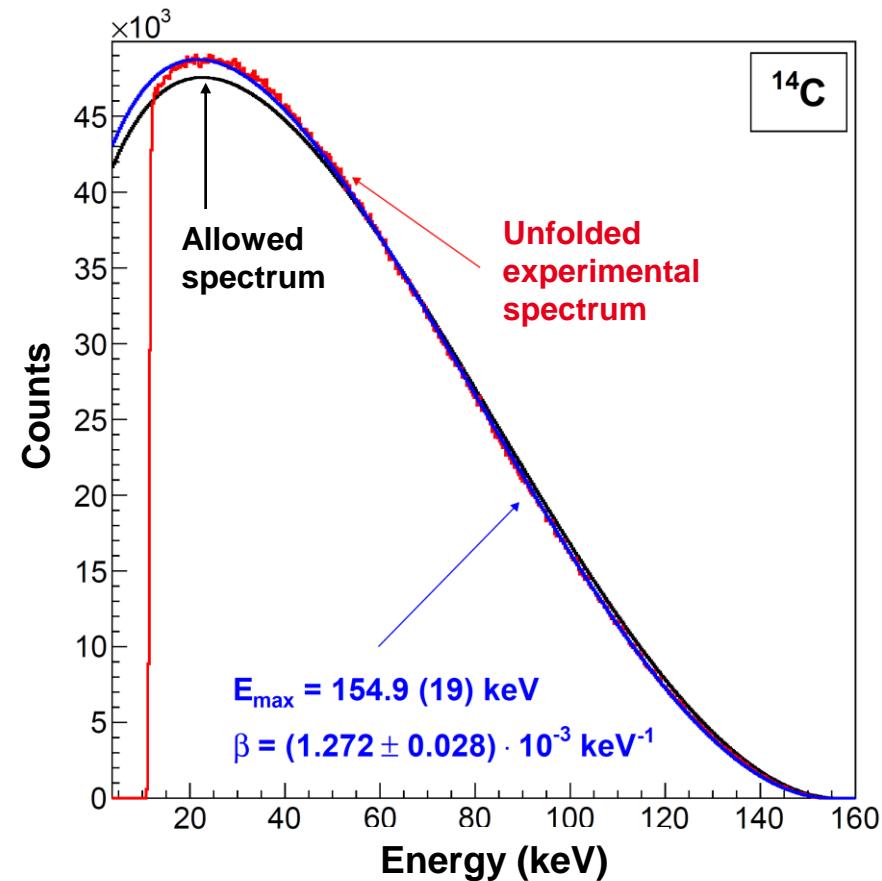
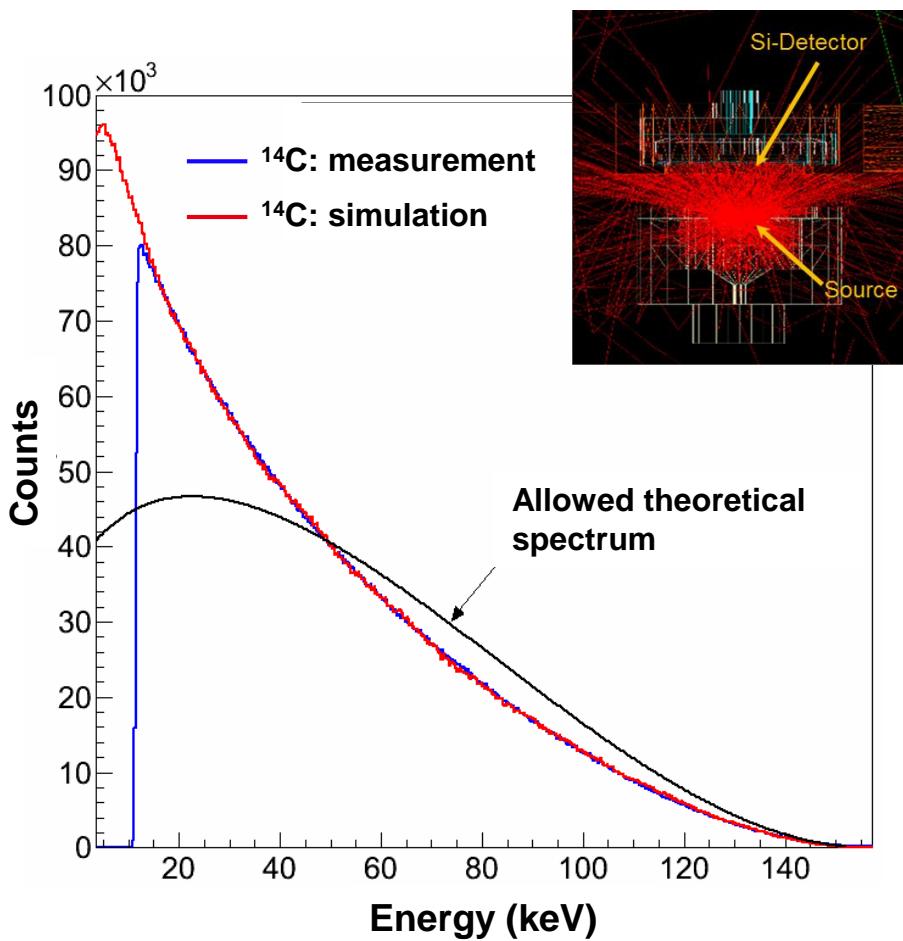
System cooled down to 10 mK

M. Loidl *et al.*, App. Radiat. Isot. 134, 395 (2018)



Single silicon detector

Charlène Bisch (PhD 2011-2014)



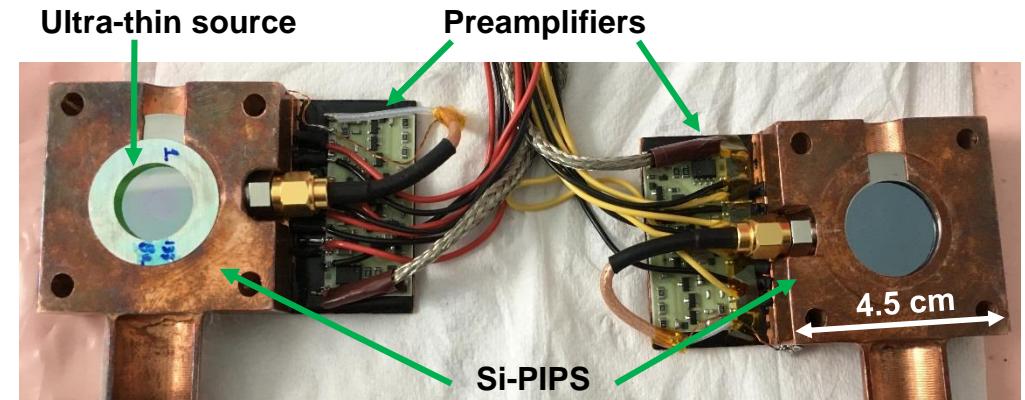
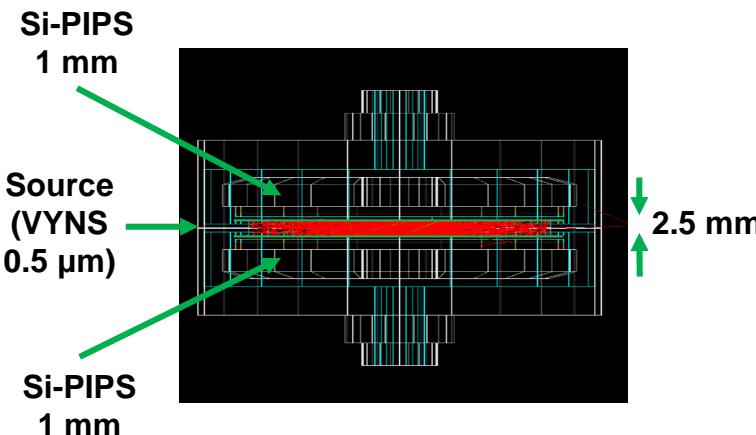
Experimental shape factor
 $C(E) = 1 + \beta(E_{\max} - E)$

Excellent
agreement with

Kuzminov, *Physics of
Nuclei*, 63 (7) (2000)

Quasi 4π geometry

Abhilasha Singh (PhD 2017-2020)

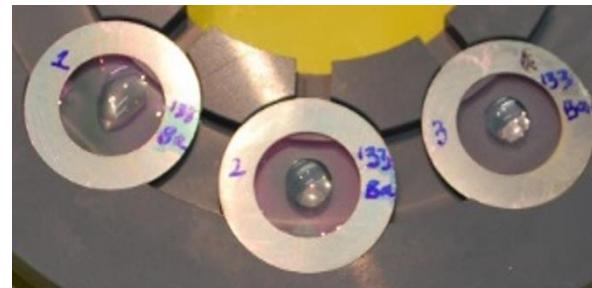


Configuration for measurement

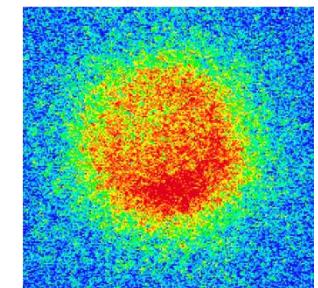


Cold finger for liquid nitrogen

Specific source preparation technique



Radioactive deposit

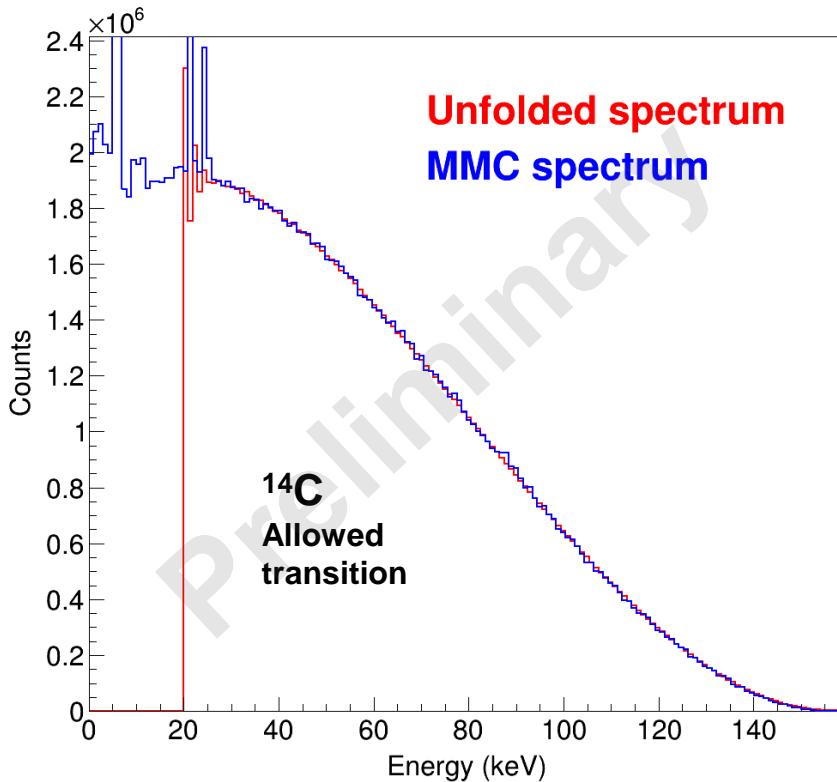


Autoradiography

- Unsealed sources: 0.5 to 0.7 μm thick
- Sealed sources: 1 to 1.5 μm thick
- Typical activity: ~1 kBq

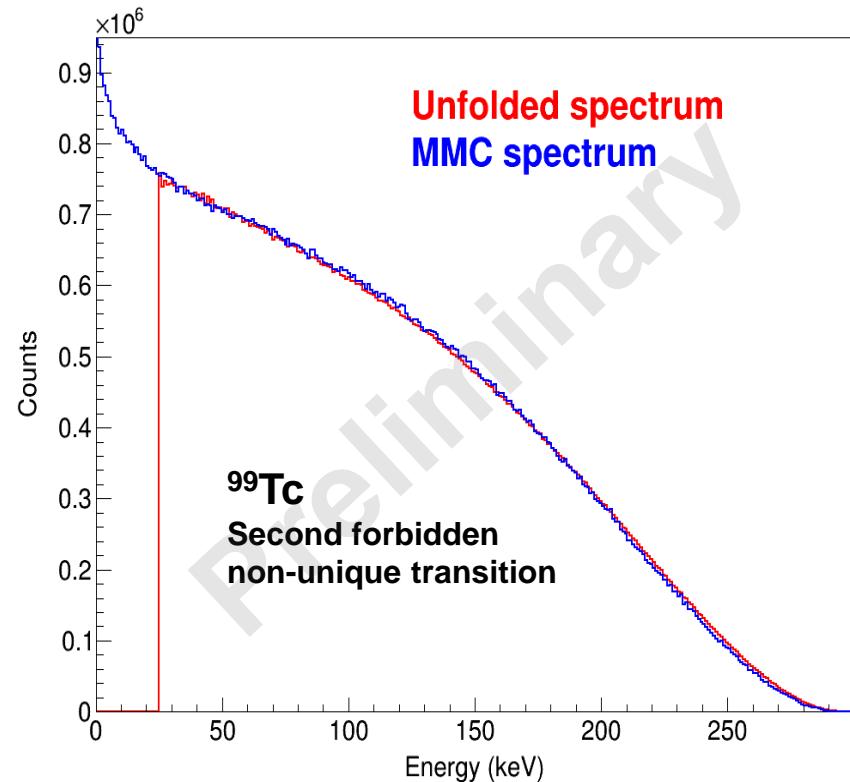
Measurements of ^{14}C and ^{99}Tc spectra

Unfolding process for silicon measurements: response matrix built from precise Monte Carlo simulations.



→ Spectrum much closer to allowed shape than in

Kuzminov, *Physics of Nuclei*, 63 (7) (2000)



→ Not consistent with existing measurement below 100 keV

Reich, Schüpferling, Z. Physik 271, 107 (1974)

Perspectives

Future work included in different projects

French metrology (2021-2024)

- Scientific Committee highlighted the importance of diffusing BetaShape. Funding of a Mac computer is ensured. Executables should be made available in 2021.
- Tabulation of atomic exchange effect for allowed and forbidden unique transitions.

European EMPIR project MetroMMC (2018-2021)

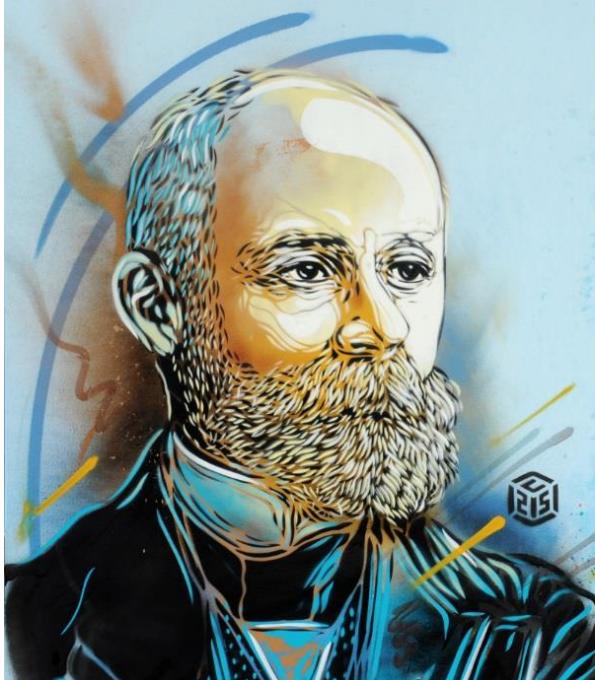
Development of a DFT code for precise atomic wave functions (CNRS). Coupling with a specific version of BetaShape done. Tests in progress.

European EMPIR project PrimA-LTD (2021-2024)

High-precision measurement and calculation of ^{55}Fe and ^{129}I decays. Nuclear structure from HFB + pnQRPA large-scale calculations.

French ANR (National Research Agency) project bSTILED (2021-2024)

PI: Oscar Naviliat-Cuncic (LPC Caen, France). High-precision measurement of ^6He spectrum for the search of tensor interactions in beta decay.



Thank you for your attention

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